Inelastic Deformation in Shock Loaded HMX

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In previous editions of T-Division Highlights we summarized calculations of equilibrium thermophysical and elastic mechanical properties of liquid and crystalline HMX. (As with the present report, we described work in progress; full details can be found in the literature.) These results, obtained using atomistic molecular dynamics (MD) and Monte Carlo methods in conjunction with a validated, flexible force field, have found a significant audience within T-Division as well as in other organizations at the Laboratory and elsewhere.

We have extended these equilibrium studies to large-scale MD calculations of the inelastic mechanical response of HMX crystal subjected to shock loading. The purpose of these nonequilibrium studies is to obtain a fundamental description of the mechanisms by which dissipation and inelastic deformation (plasticity) occurs in complicated, anisotropic polyatomic molecular crystals. The practical focus is on weak shocks, relevant for instance to accidental initiation phenomena. Indeed, the long-term goal of these studies is the development of constitutive models for plastic-bonded explosive constituent materials, for use within mesoscale simulation studies of energetic materials formulations.

We impose three major requirements on the present effort: 1) that the simulations treat a piece of material sufficiently large to capture the underlying physics without fear of severe contamination by finite-size effects; 2) that the simulations are sufficiently long to allow that physics to be revealed; and 3) that the simulations are performed for loading scenarios of direct relevance to theorists and simulators working at larger spatial scales. We have determined that three-dimensionally periodic systems containing >250,000 molecules (~7 million atoms, simulated for times of 30–100 ps are required to satisfy the first two requirements for the dynamic loading conditions of interest, namely shocks of up to only a few GPa in strength. Such calculations are only now becoming possible and, even then, only with access to substantial parallel computing resources and efficient parallel computer code. The simulations described here were performed using 128, 256, or 384 processors on the FLASH opteron cluster in conjunction with a version of the LAMMPS computer code modified to treat shockwave boundary conditions.

We focus here on a shock with $U_p = 0.5$ km/s directed along the (100) direction in the orthotropic material α-HMX. Snapshots of the material at time = 32 ps are shown in Fig. 1.

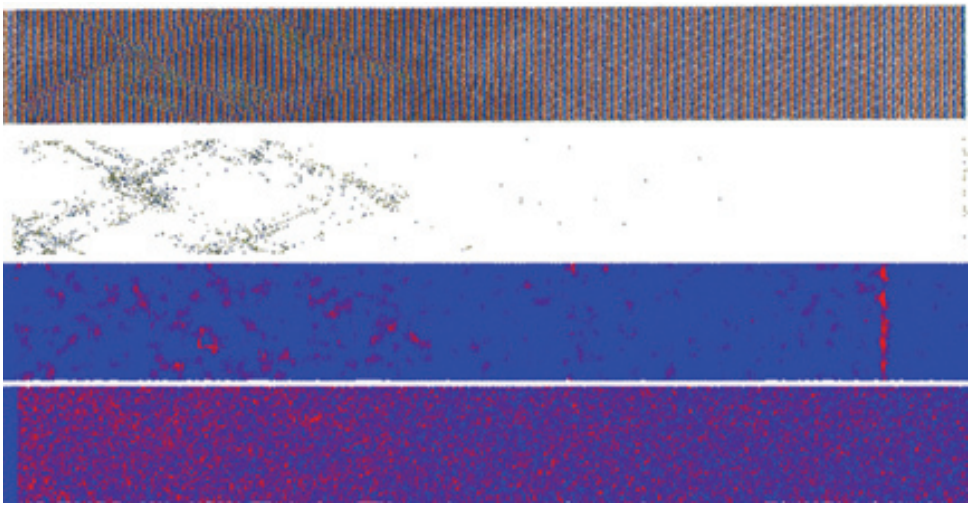

Fig. 1.
Snapshots taken during a shock in α HMX with particle velocity 0.50 km/s at time t = 32 ps. The top panel shows the position of the center of mass of the molecules, the second panel shows the molecules that have changed conformation during the simulation, and the last two panels show temperature maps for internal and local temperatures (see text for explanations).

This is a time close to breakout for the shockwave, which is propagating from left to right in the figure. Although all atoms were included in the simulation, only the molecular centers of mass are shown here for ease of presentation (thus, the twenty eight atom HMX molecule is rendered as a spherical chicken!); likewise, the coloring scheme was chosen to highlight the crystal structure present in the material at the beginning of the simulation. It is clear from the upper panel of Fig. 1 that the material has undergone localized plastic deformation, and that the mechanism by which it has done so is slip along well-defined planes in the material; dislocations in which molecular displacements by several lattice spacings are evident. It is also important to note the existence of a two-wave structure: the elastic wave associated with elastic compression at the shock front is well ahead of the plastic wave associated with inelastic deformation — dislocations and slip — in the material.

HMX contains an eight-member ring that can exist in several distinct energy minima separated by small barriers. We show in the second panel of Fig. 1 only those molecules whose conformation is different from those at t = 0, that is, those that have undergone a conformational transition. At this instant, only 0.4% of the molecules have undergone a transition, and those that have are highly correlated with the slip planes in the material. (A transient population is also observed at the shock front, but almost all of those molecules recover the starting conformation once the initial shock has passed by. We show in the bottom two panels of Fig. 1 temperature maps in the material for the "local" and "internal" temperatures, respectively. The local temperature is a measure of the relative center-of-mass velocities in a given neighborhood, whereas the internal temperature is a measure of the molecular vibrational kinetic energy.

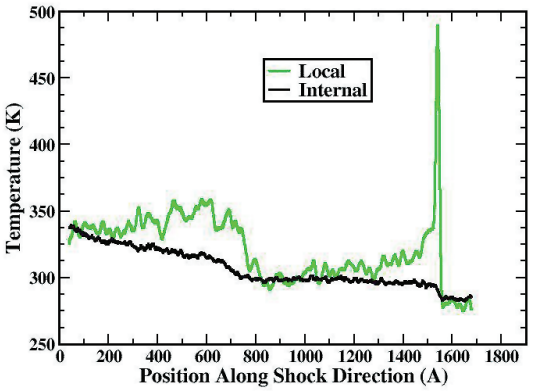

Fig. 2.
Average local and internal temperatures as a function of position for a shock in α HMX with particle velocity 0.50 km/s at time t = 32 ps.

The local temperature clearly reveals the shock front, due to the large center-of-mass acceleration as the shock passes through the material. Immediately behind the shock, the local temperature in the elastically compressed material remains relatively low. The onset of plastic deformation is clearly correlated with localization of local temperature. By contrast, the shock front is not obvious in the internal temperature map and significant molecular vibrational heating is not readily apparent until after plastic deformation has begun. This is quantified in Fig. 2, which shows the average local and internal temperatures as a function of position in the material, where the differences in magnitudes and spatial scales required for local and internal heating in the elastic and plastic waves is clearly evident.

Studies presently underway will consider the effects of varying shock strength and direction, initial temperature, material phase, and a variety of defect structures such as vacancies, voids, and grain boundaries. In addition, the distribution of local stresses in the material will be quantified to further elucidate the mechanisms of and thresholds for the onset of plastic deformation.

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